

Computational Frontier: Heterogenous Computing

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This presentation highlights advances in heterogenous computing capabilities for the Workshop on Experimental Applications of Artificial Intelligence for the Electron Ion Collider

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Modern High-Performance Computing

TITAN



Cray XK7, 18,688 Nodes 16-core AMD Interlagos + K20X 17 PFLOPS, 8.2 MW, #1 TOP500 (2012)

SUMMIT



IBM, 4,600 Nodes 2 Power9 + 6 NVidia Volta 144 PFLOPS, 9.7 MW, #1 TOP500 (2018)

FRONTIER



CRAY, 100 Cabinets
1 AMD EPYC + 4 Radeon Instinct
1.5 EXAFLOPS
Expected 2022

AND BEYOND

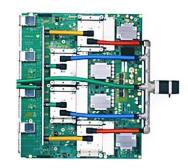


Scientific discovery and energy security depend on advances in computational capability

Modern Scientific Computing









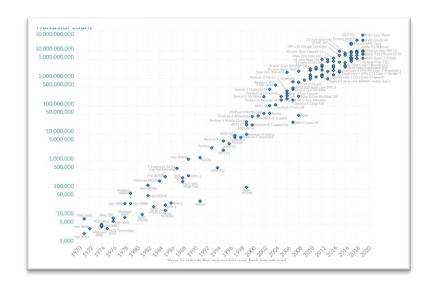


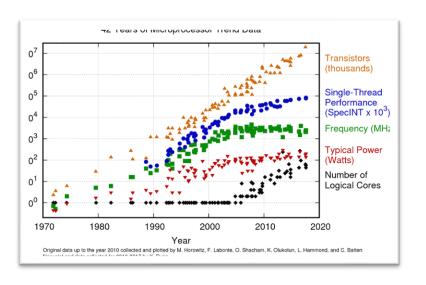




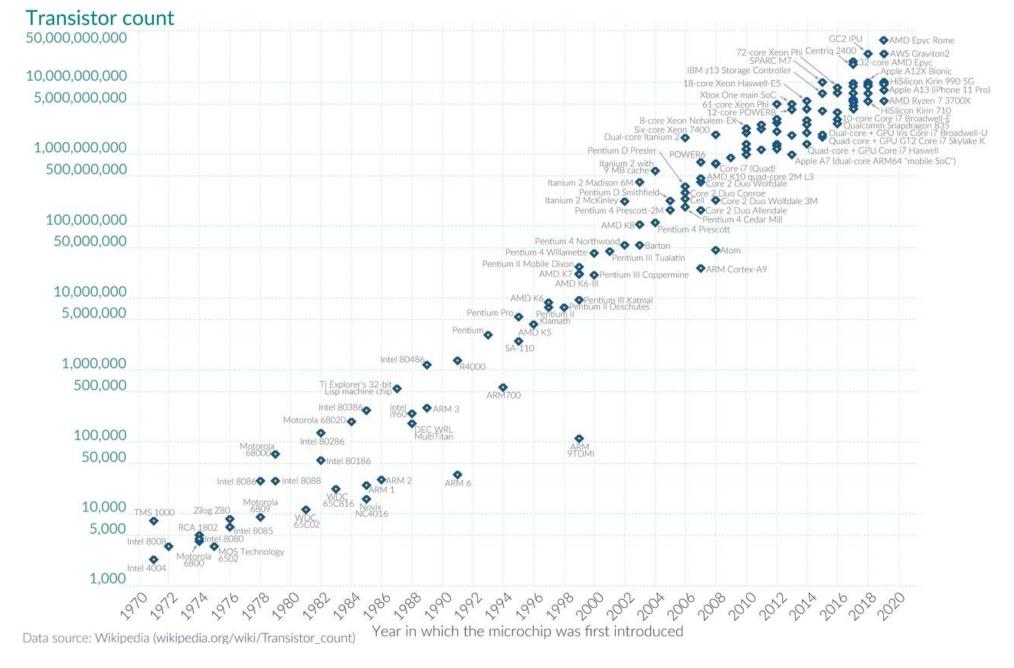
Heterogenous Computing

- In the past three decades, advances in computer technology have allowed the performance and functionality of processors to double every 2 years, i.e, Moore's law.
- The classical technological driver that has underpinned Moore's law for the past 50 years is already failing and is anticipated to flatten by 2025



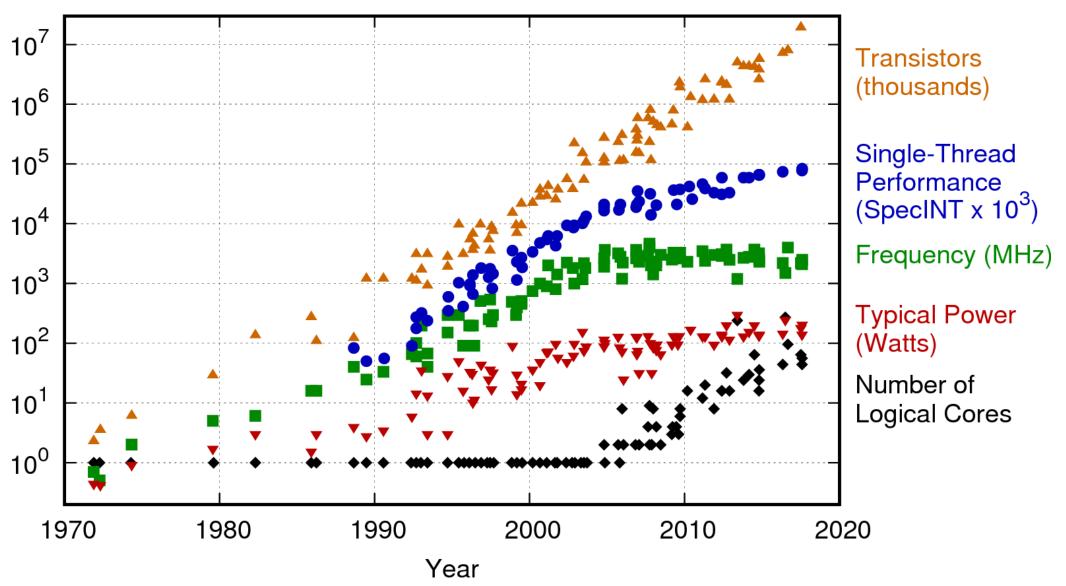








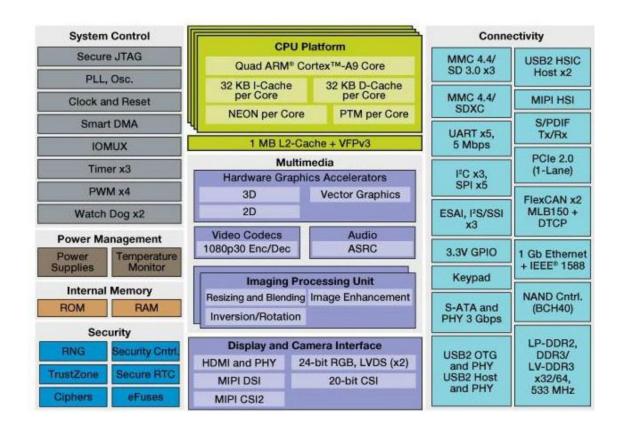
42 Years of Microprocessor Trend Data





Heterogenous Computing

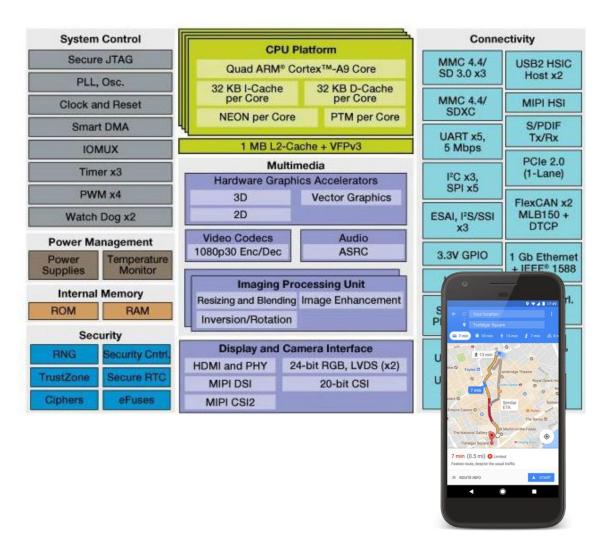
- The only tool left to a computer architect for extracting continued performance improvements is to use transistors more efficiently by specializing the architecture to the target scientific problem
- Computer vendors are pursuing systems built from combinations of different types of processors to improve capabilities, boost performance, and meet energy efficiency goals.





Heterogenous Computing

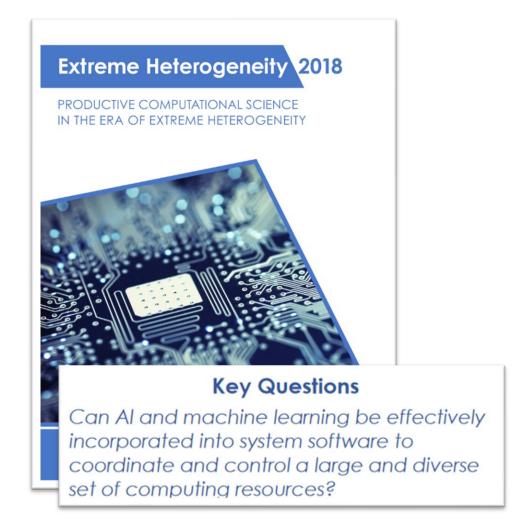
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Workshop on Productive Computational Science in the Era of Extreme Heterogeneity

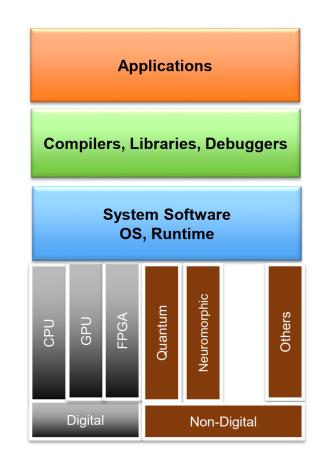
- Heterogeneity and diversity of architecture are nearly inevitable given current architecture trends
- External economic drivers and design diversity will result in systems built from a custom aggregation of components
- This fundamental change in computer architecture design has been deemed the era of "extreme heterogeneity."





Computational Science in the Era of Heterogeneity

- The difficulty and complexity of developing scientific software will increase.
- New research in computer science is needed to make future supercomputers usable, useful and secure for science applications in the 2025-2040 timeframe



Areas of Key Finds

- Programming Environments
- Software Development,
 Sustainability, and Productivity
- Operating and Runtime Systems
- Modeling and Simulation
- Facilitating Data Management,
 Analytics, and Workflows



Key Findings for Extreme Heterogeneity

- Programming Environments
 - Programmability
 - Mapping
 - Data Centricity
 - Correctness
- Software Development, Sustainability, and Productivity
 - Novel Design and Development Methodologies
 - Composability and Interoperability
 - Evolving Existing Software to New Programming Models
 - Reproducibility

- Operating and Runtime Systems
 - Design of Operating and Runtime Systems
 - Decentralized Resource Management
 - Autonomous Resource Optimization
- Modeling and Simulation
 - Methodology and Tools for Accurate Modeling of Extreme Heterogeneity
 - Cohesive Integration of Modeling and Simulation Infrastructure with Programming Environment and Runtime System
- Facilitating Data Management, Analytics, and Workflows
 - Mapping Science Workflows to Heterogeneous Hardware and Software Services
 - Adapting Workflows and Services Through Learning Approaches



Five Priority Research Directions

- 1. Maintaining and Improving Programmer Productivity
- Flexible, expressive, programming models and languages
- Intelligent, domain-aware compilers and software development tools
- Composition of disparate software component content
- 2. Managing System Resources Intelligently
- Automated methods using introspection and machine learning
- Optimize for performance, energy efficiency, and availability

- 3. Modeling and Predicting Performance
- Evaluate impact of potential system designs and application mappings
- Model-automated optimization of applications
- 4. Enabling Reproducible Science Despite Diverse Processors and Non-Determinism
- Methods for validation on non-deterministic architectures
- Detection and mitigation of pervasive faults and errors
- 5. Facilitating Data Management, Analytics, and Workflows
- Mapping a science workflow to heterogeneous hardware and software services
- Adapting workflows and services through machine learning approaches



Al Chip Landscape

https://basicmi.github.io/Al-Chip/



Western Digital.

NOKIA













Artificial Intelligence for Science

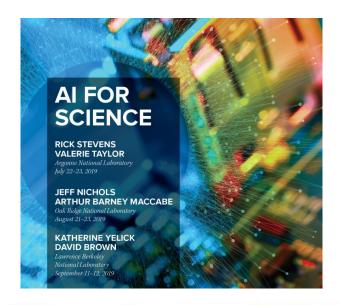
The AI for Science Town Halls so far

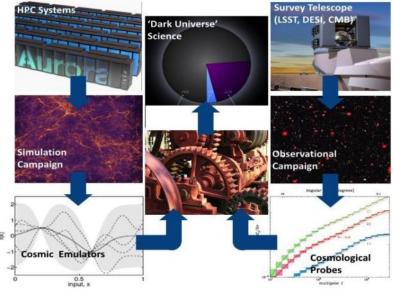
Over 1000 registrations across 4 Town Halls

+100 online	357	July 22-23	ANL
	330	Aug 20-21	ORNL
		Sept 11-12	LBNL
	273	Oct 22-23	DC
	1309	1309	Totals

- All 17 DOE National Laboratories
- 39 Companies from large and small
- Over 90 different universities
- 6 DOE/SC Offices + EERE and NNSA









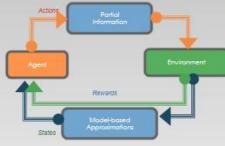
Research Challenges in Heterogenous Al

Data



- Experimental design
- Data curation and validation
- Compressed sensing
- Facilities operation and control

Learning



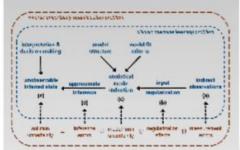
- Physics informed
- Reinforcement learning
- Adversarial networks
- Representation learning and multimodal data

Scalability



- Algorithms, complexity and convergence
- Levels of parallelization
- Mixed precision arithmetic
- Communication

Assurance



- Uncertainty quantification
- Explainability and interpretability
- Validation and verification
- Causal inference

Workflow

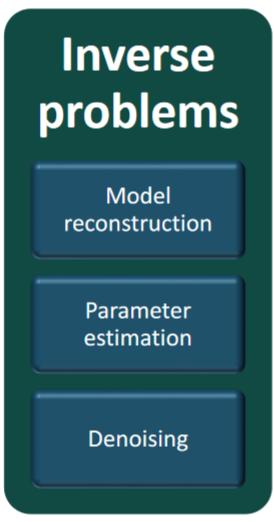


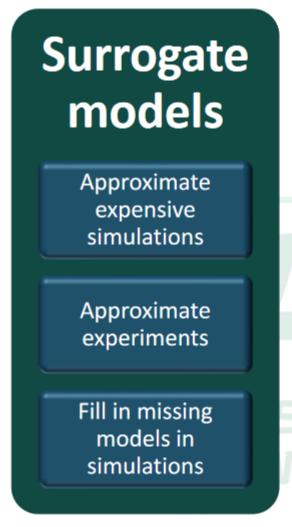
- Edge computing
- Compression
- Online learning
- Federated learning
- Infrastructure
- Augmented intelligence

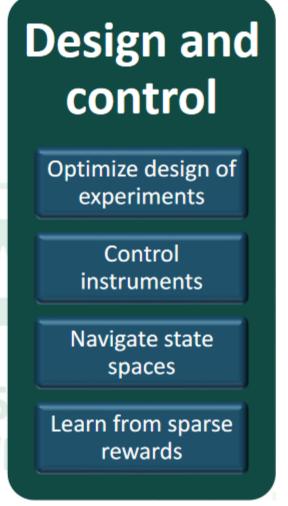


Opportunities for Artificial Intelligence



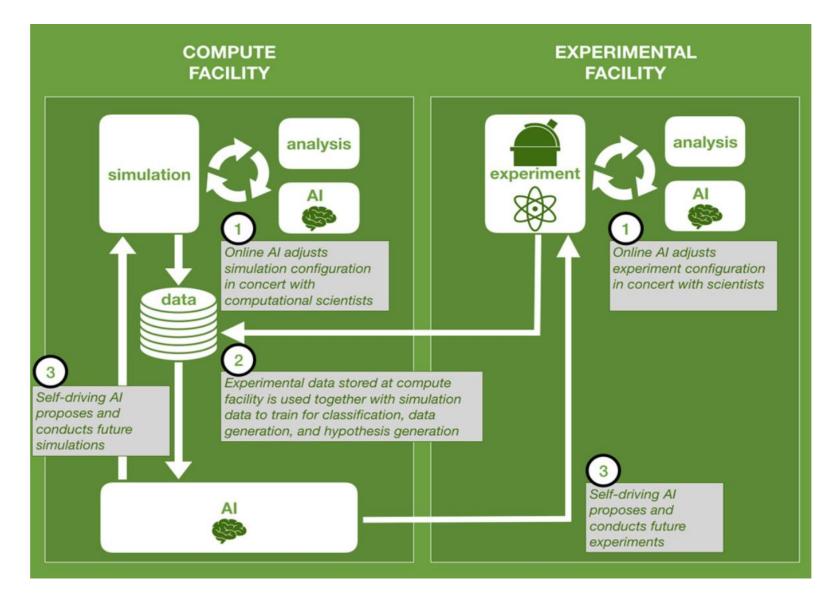






Opportunities for Artificial Intelligence

- The "inner loop" of simulations and experiments
- Accelerate and enhance traditional analysis approaches
- The "outer loop" to assist in the management and control of workflows, laboratories, and facilities.





Computational Frontier: Heterogenous Computing

- Heterogeneity and diversity of architecture are nearly inevitable given current architecture trends
- The difficulty and complexity of developing scientific software will increase.
- The opportunities of Al for Science are spurred by heterogeneous computing

Priority Research Directions

- Maintaining and Improving Programmer Productivity
- Managing System Resources Intelligently
- Modeling and Predicting Performance
- Enabling Reproducible Science Despite Diverse Processors and Non-Determinism
- Facilitating Data Management, Analytics, and Workflows

